AFRL-RX-WP-TM-2010-4128

COLLABORATIVE RESEARCH AND DEVELOPMENT (CR&D)

Delivery Order 0055: Molecular Dynamics Modeling Support

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Universal Technology Corporation

DECEMBER 2007
Final Report

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE ***(DD-MM-YY)***
December 2007

2. REPORT TYPE
Final

3. DATES COVERED ***(From - To)***
10 August 2006 – 10 December 2007

4. TITLE AND SUBTITLE
COLLABORATIVE RESEARCH AND DEVELOPMENT (CR&D)
Delivery Order 0055: Molecular Dynamics Modeling Support

5a. CONTRACT NUMBER
F33615-03-D-5801-0055

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
62102F

6. AUTHOR(S)
Timothy D. Breitzman

5d. PROJECT NUMBER
4349

5e. TASK NUMBER
L0

5f. WORK UNIT NUMBER
4349L0VT

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Universal Technology Corporation
1270 North Fairfield Road
Dayton, OH 45432-2600

8. PERFORMING ORGANIZATION REPORT NUMBER
S-531-055

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750
Air Force Materiel Command
United States Air Force

10. SPONSORING/MONITORING AGENCY ACRONYM(S)
AFRL/RXOB

11. SPONSORING/MONITORING AGENCY REPORT NUMBER(S)
AFRL-RX-WP-TM-2010-4128

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

13. SUPPLEMENTARY NOTES
PAO Case Number: 88ABW 2010-1205; Clearance Date: 16 Mar 2010. Report contains color.

14. ABSTRACT
This research in support of the Air Force Research Laboratory Materials and Manufacturing Directorate was conducted at Wright-Patterson AFB, Ohio from 10 August 2006 through 10 December 2007. We introduce a new mathematically rigorous high fidelity asymptotic theory for recovering the local field behavior inside complex composite architectures. The theory applies to zones containing strong spatial variance of local material properties. The method is used to recover the local field across ply interfaces for a pre-stressed multi-ply fiber reinforced composite. The results are shown to be in good agreement with direct numerical simulations for realistic fiber sizes and fiber- matrix elastic properties. We also demonstrate failure envelopes of composite systems using homogenization/dehomogenization micro-mechanical enhancement techniques.

15. SUBJECT TERMS
asymptotic expansion, multi-scale method, de-homogenization, failure envelope

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT:	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON (Monitor)
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**			Mark Groff
Unclassified	Unclassified	Unclassified	SAR	14	**19b. TELEPHONE NUMBER** *(Include Area Code)* N/A

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39-18

Introduction

Fiber-reinforced composites are finding use in increasing numbers of aerospace applications. One reason for this trend is that, from a structural perspective, these composites offer outstanding strength-to-weight advantages over traditional materials such as metal alloys. A common problem in composites, however, is the inability of current methods to accurately predict their strength and durability. The innate heterogeneity on the constituent level creates a complicated strain field and can create stress concentrations in the composite. The type of composites studied within is fiber reinforced composites, but the formulations extend to fully three-dimensional composites such as woven composite architectures. Because of the size and shear number of fibers in these composites, it is not practical or computationally possible to explicitly model the fiber and matrix material. Thus, homogenization methods are often used to replace the heterogeneous composite with a homogeneous block of material having representative mechanical and thermal properties. By homogenizing, however, the local details of the microstructure are lost. It is these local details that can play large roles in stress concentrations and ultimately failure of the composite. De-homogenization techniques provide the recovery of these important local details.

One type of stress concentration occurs when the microstructure changes abruptly (e.g. a ply interface). The first goal of this work was to create an analytical tool to model and predict the strain felt on the level of the microstructure in the composite where the microstructure abruptly changes.

Task 1: Formulation of the asymptotic theory for abruptly changing microstructures

It was shown in [1] that periodic homogenization methods are sufficient to predict strain states when the microstructure is uniformly periodic. Figure 1 illustrates the success of these methods on a free edge problem comprised of a 0/90/0 IM7/5250-4 composite laminate subjected to a 1% displacement strain in the 0° direction. The failure criteria J1 and J2 are dilatational and deviatoric strain invariants known in the literature as Strain Invariant Failure Theory (SIFT), introduced by Gosse et al in [2]. The curves referred to as “Ply RVE” in Figure 1 are the curves computed according to the periodic homogenization in [1] and the curves referred to as “3D Sim.” are the strain invariants computed by explicitly modeling the fiber and matrix materials.

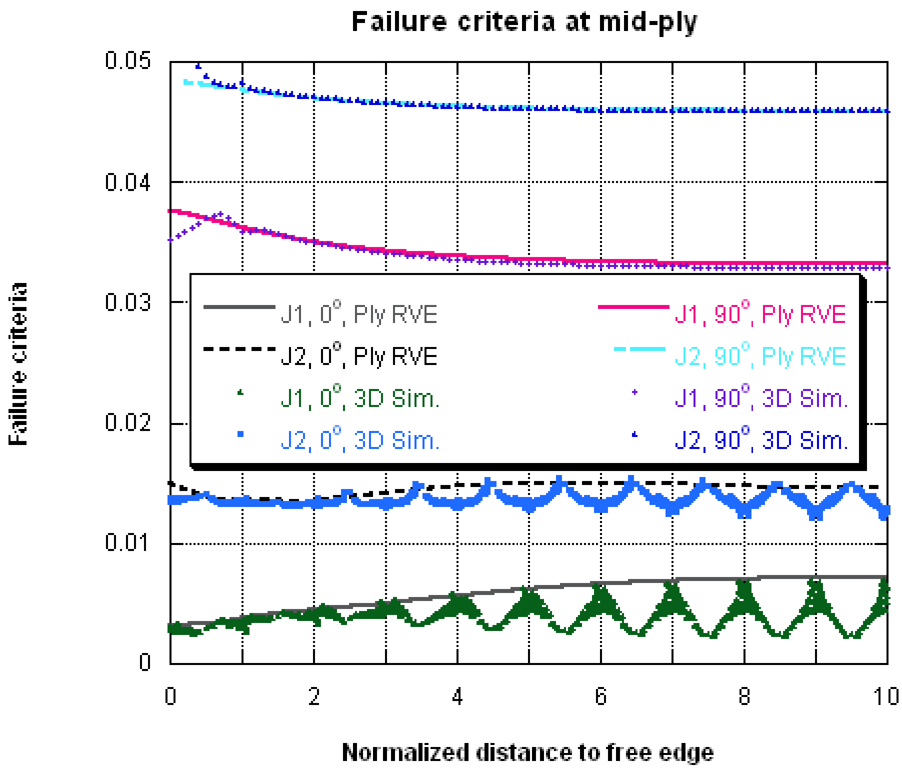

Figure 1: Plot of failure criteria versus distance to free edge at mid-ply of both the 0 and 90 degree plies

The periodic homogenization/de-homogenization methods are upper bounds on the actual strain in the explicitly modeled fiber/matrix composite, illustrating that the multi-scale methods give accurate results when the microstructure is uniformly periodic.

As one approaches the 0°/90° interface, these methods based strictly on a uniformly periodic microstructure are no longer able to capture the trends of the explicitly modeled solution. Figure 2 and Figure 3 show the strain invariant plots 0.5 fiber diameters above the ply interface. Note in Figure 3 how the second strain invariant in the full numerical simulation exceeds the bound from the multi-scale bound prediction assuming uniformly periodic microstructure. It is not surprising that problems would arise in this region since the microstructure shifts abruptly from a 0° fiber geometry to a 90° fiber geometry.

To fix ideas for the asymptotic theory near a ply interface, we illustrate the approach for a pre-stressed laminate made up of several plies with each ply containing a different periodic array of fibers. We focus on a domain of interest ``S'' inside the composite. The characteristic length of the fiber size and spacing relative to the length scale of the laminate is given by ε. A domain of interest containing the interface between two plies is shown in Figure 4. The elastic displacement and strain inside the composite laminate are written as u^{ε} and e^{ε} respectively. Next we replace the local elastic properties inside each ply with the effective elastic tensor associated with each ply. We then consider the elastic strain field $e^{H}(x)$ associated with the laminate composed of plies

modeled by their effective elastic stiffness properties. The new high fidelity asymptotic representation for the actual strain inside the domain of interest S is given by

$$e^{\varepsilon}(x) = P^{\varepsilon}(x)e^{H}(x) + e(\eta^{\varepsilon}(x))+)(\varepsilon)\,, \tag{1}$$

where the tensor valued function P^{ε} and vector field η^{ε} are determined by local boundary value problems formulated over the domain of interest S. The tensor P^{ε} is computed in terms of the local elastic fluctuation $w^{\varepsilon,ij}$ that is periodic on S and solves

$$div(C^{\varepsilon}(x)(e^{\varepsilon,ij}(x) + e^{ij}) = div(C^{E}(x)e^{ij}). \tag{2}$$

Here, the effective elasticity tensor for each ply is given by $C^{E}(x)$, the local elastic property for the fiber and matrix phase is given by $C^{\varepsilon}(x)$, $e^{ij}_{kl}=\delta_{ik}\delta_{jl}$ and $e^{\varepsilon,ij}$ is the local strain inside S is associated with $w^{\varepsilon,ij}$ and

$$P^{\varepsilon,ij}_{kl}(x) = e^{\varepsilon,ij}_{kl}(x) + e^{ij}_{kl}. \tag{3}$$

The field η^{ε} is periodic on S and captures the local strain fluctuation due to pre-stress. The local stress free strain takes different values inside fiber and matrix phases and is denoted by e^{ε}. The function η^{ε} is the solution of

$$div(C^{\varepsilon}(x)(e(\eta^{\varepsilon}) + e^{\varepsilon}(x)) = div(H^{E}(x))\,, \tag{4}$$

where the effective thermal expansion coefficient for each ply is given by $H^{E}(x)$ and $e(\eta^{\varepsilon})$ is the strain associated with η^{ε}. Here it is noted that all differential equations are interpreted in the weak sense.

Figure 5 illustrates the results of the new asymptotics applied to the previous 0/90/0 free edge problem. The smooth, black lines indicate the full numerical simulation explicitly modeling the fiber an matrix phases, the dashed, blue lines portray the bound from the uniformly periodic microstructure asymptotics, and the dotted red line displays the bound using the new interface asymptotics. It is clear that the previous bound is exceeded by the full simulation, while the new interface bound models the behavior quite well. This work was submitted for publication to the SIAM Journal of Multiscale Modeling & Simulation in October, 2006.

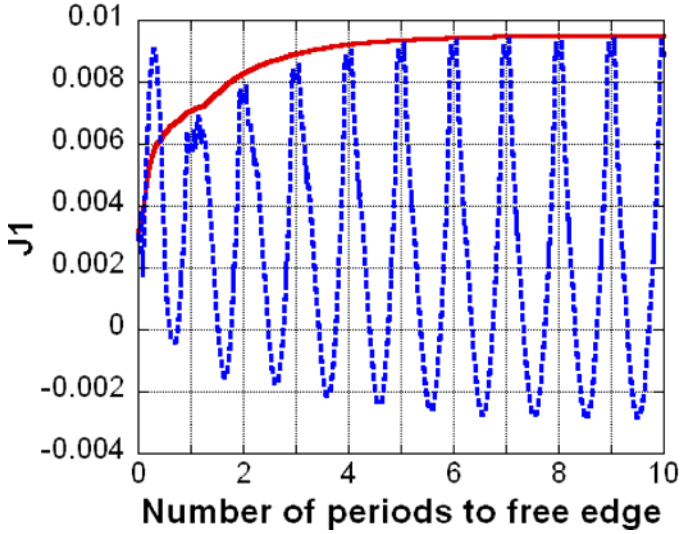

Figure 2: Plot of dilatational strain invariant 0.5 fiber diameters above ply interface

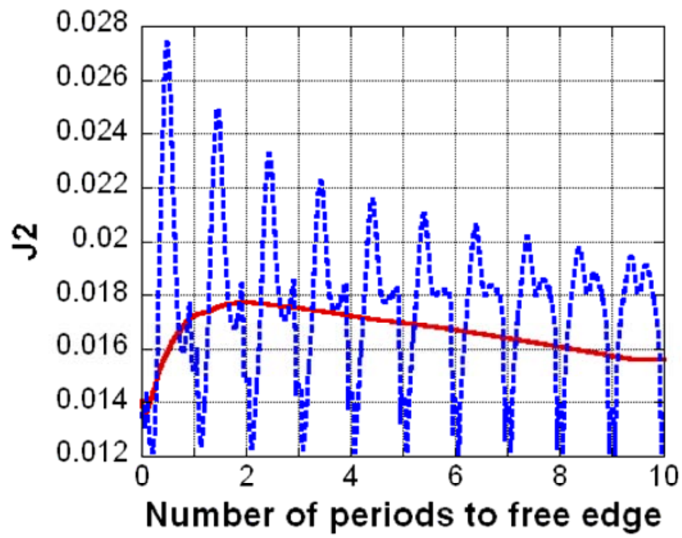

Figure 3: Plot of deviatoric strain invariant 0.5 fiber diameters above ply interface

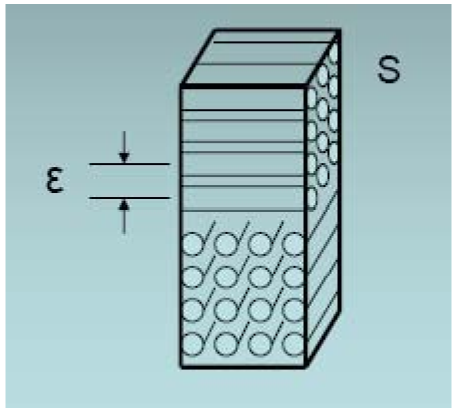

Figure 4: Domain of interest containing the interface between two plies with fiber orientation at 0 and 90 degrees.

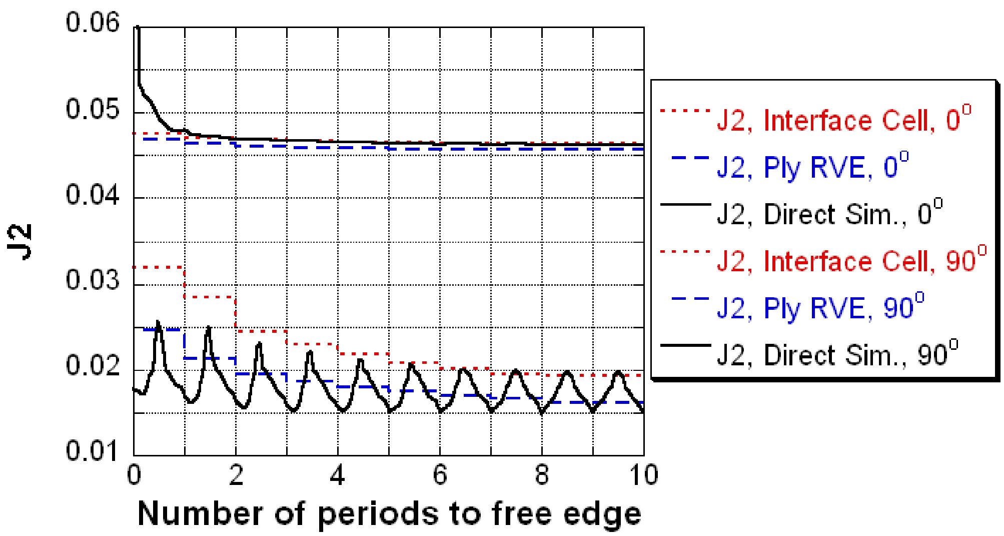

Figure 5: Deviatoric strain invariant at ply interface

Task 2: Comparison of failure criteria for the fiber/matrix level

This task was not originally planned to be a part of the work. After the interface issue was addressed, the focus was to optimize the fiber orientation angles for a scarf repair patch. Before we proceeded with the optimization routine, however, we had to pick a failure criteria to use on the micro level (level of the fiber and matrix). We used two micro level failure criteria in this study. The first was stress invariants in which the dilatational and deviatoric critical values were deemed independent of each other. In other words, no interaction was assumed between the two failure modes. Second, we used the criteria for metal yielding by Doyoyo and Wierzbicki [3]. We note that the Raghava criterion ([4]) is exactly equal to the Doyoyo-Wierzbicki criterion with the shape parameter η set equal to one.

Failure envelopes were computed for two different material systems under different loading conditions. The first comparison between the failure criteria was an in-

plane shear-transverse tension test on E-Glass/LY556 composite. For calibration of the stress invariant criteria (S-I), we used 90° transverse tension to back out the critical dilatational invariant value. The critical deviatoric invariant was determined by pure shear on a 90° specimen. For the Doyoyo-Wierzbicki criterion (D-W), we calibrated by pure tension and pure compression on the 90° specimen, then adjusted the η parameter to match the shear point. Figure 6 displays the experimental and predicted failure envelopes of the E-glass/LY556 composite. Experimental data was taken from [4,5]. Predictions were done with and without prestress. Because of the low stress-free temperature of the composite, little difference is seen in the analytical predictions with and without prestress. It is clear, however, that the independence of the failure in the stress invariant criteria leads to a poor prediction in the shear-tension regime. The DW criterion appears to capture the trend much more accurately.

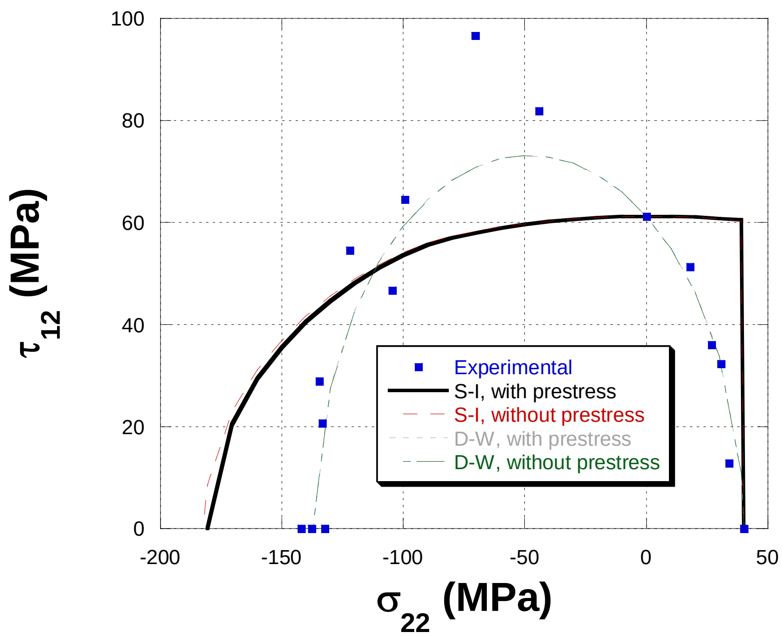

Figure 6: Tension/shear failure envelope of E-glass/LY556 composite

The second failure predictions were made for AS4/3502 angle-ply composites loaded under compression. Experimental data was obtained from [6]. The critical dilatational invariant value for the stress invariant criteria was obtained from a transverse tension test. The deviatoric critical value was taken from the ±45 angle ply under compression. Calibration for the Doyoyo-Wierzbicki criterion was accomplished using the 90 degree specimen under tension and compression. The η parameter was then adjusted to match the ±45 angle ply experimental data. Once again, predictions were made with and without prestress. The AS4/3502 composite has a larger stress-free temperature than the E-glass/LY556 composite, thus differences between the predictions are not negligible in this case.

Figure 7 displays the experimental results and analytical predictions of the angle ply data. It is clear that the D-W criterion performs better than the stress invariant criteria. It should be noted, however, that neither criteria accurately capture the trend once the ply angles are smaller than 30 degrees. It is believed that inside 30 degrees,

other failure modes (such as fiber buckling) are affecting the laminate failure. The D-W criterion with prestress shows a marked improvement over the D-W prediction without prestress on the ±60 degree specimen.

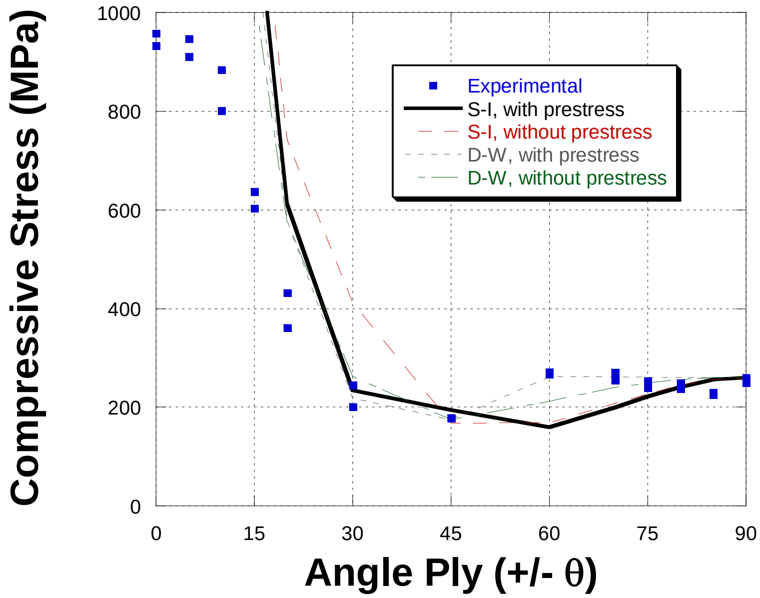

Figure 7: Failure of AS4/3502 angle ply laminates

Conclusion

We note that, at present, we have not optimized the ply angles for the scarf joint. The micromechanical failure criteria study points us toward interactive criteria for predicting failure in the matrix phase of the composite. Although the Doyoyo-Wierzbicki criterion appears promising as a micro-level failure criterion, more validation is needed to test the situational robustness of the criterion.

We conclude by pointing out that the convergence implied by (1) holds for points inside the prescribed domain of interest S. The new asymptotic theory shows that the approximation improves when the length scale of the heterogeneity is small relative to the domain of interest. Heuristically this implies that the approximation improves if the size of the domain of interest is ``large enough'' with respect to the heterogeneity. One can think of the domain of interest as being a particular choice of Representative Volume Element (RVE). The question of selecting the proper RVE size for deterministic and random media is an active area of investigation [7,8] and has direct impact on the choice of local enhancement of the FEM seen in multi-scale numerical methods [9-17]. The framework given by the asymptotic expansion (1) provides a new mathematical context for the investigation of the effect of the location and size of the RVE on the fidelity of the approximation and choice of FEM enrichment for multi-scale numerical methods.

References

[1] Breitzman, T.D., *Multi-scale strain analysis*, Ph.D. dissertation, Louisiana State University, 2005.

[2] Gosse, J.H., and Christensen, S., 42^{nd} AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference and Exhibit Technical Papers, Apr 16-19 2001, vol. 1, pp. 45-55.

[3] Doyoyo, M., and Wierzbicki, T., International Journal of Plasticity, vol. 19, 2003, pp. 1195-1214.

[4] Soden, P.D., Hinton, M.J., and Kaddour, A.S., Composites Science and Technology, vol. 58, 1998, pp. 1011-1022.

[5] Doden, P.D., Hinton, M.J., and Kaddour, A.S., Composites Science and Technology, vol. 62, 2002, pp. 1489-1514.

[6] Shuart, M.J., AIAA Journal 27, 1989, pp. 1274-1279.

[7] Swaminathan, S., Ghosh, S., and Pagano, N.J., Journal of Composite Materials, vol. 40, 2006, pp. 605-622.

[8] Jiang, M., Ostoja-Starzewski, M., and Jasiuk, I., J. Mech. Phys. Solids, vol. 49, 2001, 655-673.

[9] Aboudi, J., Pindera, M.-J., and Arnold, S.M., CPSOA, Part B-Engineering, vol. 30, 1999, pp. 777-832.

[10] Ming, W.E.P., and Zhang, P., Journal of the American Mathematical Society, vol. 18, 2004, pp. 121-156.

[11] Efendiev, Y.R., Hou, T.Y., and Wu, X., J Comput. Phys., vol. 37, 2000, pp. 888-910.

[12] Fish, J., Yuan, Z., Hou, T.Y., and Wu, X., Int. J. Mum. Meth. Engr., vol. 62, 2005, pp. 1341-1359.

[13] Hou, T.Yl, and Wu, X.H., Journal of Computational Physics, vol. 134, 1997, pp. 169-189.

[14] Hou, T.Y., Wu, X.H., and Cai, Z., Mathematics of Computation, vol. 227, 1999, pp. 913-943.

[15] Oden, J.T., Vemaganti, K. and Moes, N., Comput. Methods Appl. Mech. Engng., vol 172, 1999, pp. 3-25.

[16] Oden, J.T. and Zohdi, T.I., Comput. Methods Appl. Mech. Engng., vol. 148, 1997, pp. 367-391.

[17] Strouboulis, T., Zhang, L. and Babuska, I., Int. J. Num. Meth. Engr., vol. 60, 2004, pp. 1639-1672.